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High pressure liquid densities and excess volumes of the (di-isopropyl ether + 1-hexanol) system

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ABSTRACT

New experimental density data for binary mixtures of (di-isopropyl ether + 1-hexanol) over the composition range are reported, between 293.15 and 393.15 K, and for pressures from 0.1 MPa up to 140 MPa. To perform these measurements, a vibrating tube densitometer, calibrated with an uncertainty of ±0.35 kg·m^{-3} was used. The experimental density data were fitted with a Tait-like equation. From experimental data, excess volumes have been calculated as well as the isobaric thermal expansivity and the isothermal compressibility have been derived from the Tait-like equation.

1. Introduction

The scarcity and costs associated with petroleum reserves make the use of biofuels coming from renewable energy resources more attractive, as declared by international legal acts [1,2]. Amongst renewable biofuels, those containing oxygenated compounds are the best candidates for new fuels in automotive engines [3]. The biggest advantage that biofuel has over petroleum gasoline and diesel is its environmental friendliness [4].

During the last three decades, various ethers, either alone or in mixture with other ethers or alcohols, have been widely used to reduce pollutant emissions [5–9]. Di-isopropyl ether (DIPE), as branched alkyl ether, has been considered as a potential biofuel due to its important advantages from the environmental point of view, as low solubility in water, non-toxicity and non-polluting properties [10–12].

This work presents the experimental densities of the system (DIPE + 1-hexanol) at pressures from (0.1 to 140) MPa and temperatures from (293.15 to 393.15) K over the full composition range. In previous works [13,14], we have studied high pressure and high temperature density of DIPE and 1-hexanol as pure compounds. Previous measurements on density of the mixture were reported by [7] at 0.1 MPa and 298.15 K. We report densities, excess molar volumes, isobaric thermal expansion coefficient and the isothermal compressibility coefficient for the binary mixtures (DIPE + 1-hexanol) at high pressures and temperatures.

2. Experimental

2.1. Materials

Di-isopropyl ether and 1-hexanol were obtained from Sigma-Aldrich with mole fraction purity of 0.995, as shown in Table 1. Both liquids were stored over a molecular sieve to avoid any moisture and were used without any further purification except careful degassing before the use. Content of water of 1-hexanol was checked by means of a Mettler Toledo C20 coulometric Karl Fischer titrator.

2.2. Measurement technique. Experimental procedure

Liquid mixtures were prepared by weighing, with an estimated standard uncertainty in the mass fraction of $\pm 5 \times 10^{-4}$. A Sartorius CP 224 S balance was used with an accuracy of $\pm 1 \times 10^{-4}$ g. Prior to measurements, pure substances were degassed using a Branson 3210 ultrasound bath for at least 15 min at room temperature.

The densities were measured using an Anton Paar DMA HPM vibrating-tube densitometer described in detail previously [15]. This model is suitable for the high accurate determination of

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Table 1
Purity and related data for the chemicals studied.

Compound	Molecular formula	Molar Mass/(g·mol^{-1})	Mole fraction purity (stated)[a]	CAS number
DIPE	$C_6H_{14}O$	102.17	0.995	108-20-3
1-Hexanol	$C_6H_{14}O$	102.17	0.995[b]	111-27-3

[a] Determined by gas chromatography (GC) by the supplier Sigma Aldrich.
[b] The water content was checked to be less than 0.01 (mol%) by titration method.

Table 2
Experimental densities, ρ/(g·cm^{-3}), for x DIPE + $(1-x)$ 1-hexanol at various temperatures T and pressures p.[a]

x	p/MPa	T/K					
		293.15	313.15	333.15	353.15	373.15	393.15
ρ/g·cm^{-3}							
0.1524	0.1	0.8067	0.7915	0.7756	0.7592	0.7418	
	0.5	0.8069	0.7918	0.7760	0.7595	0.7420	0.7247
	1	0.8072	0.7922	0.7765	0.7600	0.7426	0.7254
	2	0.8079	0.7930	0.7774	0.7610	0.7438	0.7267
	5	0.8100	0.7953	0.7800	0.7640	0.7471	0.7305
	10	0.8134	0.7990	0.7842	0.7687	0.7524	0.7366
	15	0.8166	0.8026	0.7881	0.7731	0.7573	0.7421
	20	0.8197	0.8060	0.7918	0.7773	0.7619	0.7473
	30	0.8257	0.8124	0.7988	0.7850	0.7705	0.7567
	40	0.8312	0.8185	0.8054	0.7920	0.7782	0.7653
	50	0.8363	0.8239	0.8113	0.7985	0.7852	0.7728
	60	0.8413	0.8293	0.8170	0.8046	0.7918	0.7799
	70	0.8461	0.8343	0.8224	0.8103	0.7979	0.7867
	80	0.8504	0.8390	0.8273	0.8157	0.8038	0.7928
	90	0.8547	0.8434	0.8322	0.8208	0.8092	0.7986
	100	0.8588	0.8478	0.8368	0.8257	0.8143	0.8041
	110	0.8627	0.8520	0.8411	0.8304	0.8194	0.8094
	120	0.8665	0.8559	0.8455	0.8349	0.8242	0.8144
	130	0.8703	0.8599	0.8494	0.8391	0.8286	0.8191
	140	0.8737	0.8636	0.8534	0.8432	0.8330	0.8237
0.3196	0.1	0.7921	0.7760	0.7592	0.7417	0.7233	
	0.5	0.7923	0.7763	0.7596	0.7421	0.7235	0.7050
	1	0.7927	0.7767	0.7601	0.7427	0.7241	0.7057
	2	0.7935	0.7776	0.7611	0.7438	0.7255	0.7073
	5	0.7957	0.7802	0.7640	0.7471	0.7292	0.7117
	10	0.7995	0.7843	0.7687	0.7524	0.7353	0.7187
	15	0.8030	0.7882	0.7730	0.7573	0.7408	0.7249
	20	0.8064	0.7919	0.7771	0.7619	0.7459	0.7307
	30	0.8128	0.7989	0.7848	0.7704	0.7554	0.7411
	40	0.8186	0.8054	0.7919	0.7780	0.7638	0.7504
	50	0.8241	0.8112	0.7983	0.7850	0.7713	0.7586
	60	0.8294	0.8170	0.8044	0.7916	0.7784	0.7664
	70	0.8345	0.8223	0.8101	0.7977	0.7849	0.7735
	80	0.8391	0.8273	0.8154	0.8033	0.7912	0.7799
	90	0.8436	0.8320	0.8204	0.8089	0.7969	0.7861
	100	0.8480	0.8366	0.8253	0.8140	0.8024	0.7918
	110	0.8520	0.8410	0.8298	0.8189	0.8076	0.7975
	120	0.8560	0.8452	0.8344	0.8236	0.8126	0.8027
	130	0.8599	0.8492	0.8386	0.8280	0.8173	0.8076
	140	0.8635	0.8532	0.8428	0.8324	0.8218	0.8124
0.4906	0.1	0.7763	0.7591	0.7411	0.7225	0.7027	
	0.5	0.7767	0.7595	0.7416	0.7230	0.7031	0.6835
	1	0.7771	0.7600	0.7422	0.7236	0.7039	0.6844
	2	0.7779	0.7610	0.7433	0.7249	0.7054	0.6863
	5	0.7804	0.7639	0.7467	0.7288	0.7099	0.6915
	10	0.7845	0.7684	0.7518	0.7348	0.7167	0.6995
	15	0.7883	0.7727	0.7567	0.7402	0.7230	0.7066
	20	0.7920	0.7768	0.7612	0.7453	0.7288	0.7132
	30	0.7990	0.7843	0.7696	0.7546	0.7391	0.7247
	40	0.8053	0.7914	0.7773	0.7629	0.7484	0.7350
	50	0.8112	0.7977	0.7842	0.7705	0.7566	0.7439
	60	0.8168	0.8038	0.7907	0.7776	0.7642	0.7522
	70	0.8221	0.8095	0.7968	0.7842	0.7713	0.7599
	80	0.8271	0.8147	0.8024	0.7901	0.7780	0.7668
	90	0.8318	0.8197	0.8078	0.7961	0.7840	0.7734
	100	0.8363	0.8246	0.8130	0.8015	0.7898	0.7795
	110	0.8406	0.8292	0.8178	0.8067	0.7953	0.7854
	120	0.8448	0.8336	0.8226	0.8116	0.8006	0.7908
	130	0.8489	0.8378	0.8270	0.8163	0.8055	0.7960